Abstract for an Invited Paper for the 1996 March Meeting of the American Physical Society 16-20 March 1995, St. Louis, MO.

Phase Diagram of Iron at High Pressures and High Temperatures* C. S. YOO, Lawrence Livermore National Laboratory, Livermore, CA.

The magnetic properties and phase transitions of iron at high temperatures and moderate pressures are central to the behavior of technologically important iron and iron alloys. Considering the fact that iron is the dominant component of Earth's core, the phase diagram of iron at high temperatures and high pressures is also fundamental to Earth science. We have studied the phase diagram of iron to 130 GPa and 3500 K by in-situ, x-ray diffraction studies of laser-heated iron in a diamond anvil cell. The results reveal several important constraints for the phase diagram of iron. First, a new dhcp phase of iron, ε'-Fe, is found between 15 and 40 GPa. Its stability and magnetic properties have also been examined by a series of *ab-initio* total energy calculations on the hcp, dhcp, and fcc phases of iron. Second, the ε/γ /liquid triple point of iron is located at 2500 \pm 200 K and 50 ± 10 GPa, substantially lower pressure than the previous result. Third, ε-Fe is stable in a wide range of temperatures between 50 GPa and 110 GPa. No evidence was found for any other phases including β - and α '-Fe. Fourth, above 110 GPa there is an indication of new crystalline, arising either from a solid-solid transition or more likely from a chemical reaction of ε -Fe. The implications of these results for the Earth's core will also be discussed, together with the experimental issues associated with *in-situ* x-ray diffraction studies at high pressures and temperatures.

* Work performed in collaboration with J. Akella, J. Moriarty, P. Soderlind at LLNL and A. Campbell, D. Mao, and R. Hemley at Geophysics Laboratory under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract number W-7405-ENG-48.